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Notes on Uncertainty Propagation from Flux to α in Reaction History

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It is crucially important for comparison between reaction history experimental data and results of the high performance weapons simulations that all types of uncertainty are correctly captured and propagated through the process. These notes are intended to formulate the problem, to provide a general overview, and remarks on the current stage of the research.

Repeatability of an experiment and uncertainty of its measurement are separate problems, independent from each other

A golden standard in science is to repeat any given experiment a statistically significant number of times, and catch the spread of the produced results measured using the same set of detectors and the same data analysis methodology. Resulting spread of the recorded data is used to assign experimental error. In such case experimental error combines limitations on repeatability of the experiment with uncertainty created by the detectors/process of measurement.

Underground nuclear events were one of a kind experiments. This means we need to clearly differentiate between repeatability of the experiment itself, and uncertainty created by the process of measurement. They are physically independent. In general, experiments involving stochastic behaviors like chaos or turbulence create a significantly broader spread of possible outcomes than the ones that do not involve stochastic behaviors, yet no physical experiment is perfectly repeatable, ever. Uncertainty of measurement depends on quality of the detectors, and on the whole process of gathering and analyzing the data. Uncertainty of the measurement can be so large that any variation in repeatability of given experiment would be negligible in relation to uncertainty of its measurement; yet in other cases uncertainty of measurement can be orders of magnitude smaller than spread of data obtained in repetition of the same experiment. For one-of-a-kind experiments like nuclear events we need to keep in mind that only uncertainty of measurement and data analysis is discussed – it provides no information about repeatability of the experiment itself.

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In recent years attempts have been made to compare data from statistically significant number of nuclear events in the aspects in which the data can be meaningfully compared across the set. This is a promising direction for assigning an independent upper limit of uncertainty of flux measurement, and research is in progress. Such upper limit combines variation on repeatability of the experiment and uncertainty of the measurement, like in a typical scientific assignment of the experimental error. Only certain, rather limited aspects of the experiment can be compared this way. The research results will not substitute for a series of repeated identical experiments.

Comparing experimental reaction history with simulations is a process in which multiple independent types of uncertainty are created and propagated.

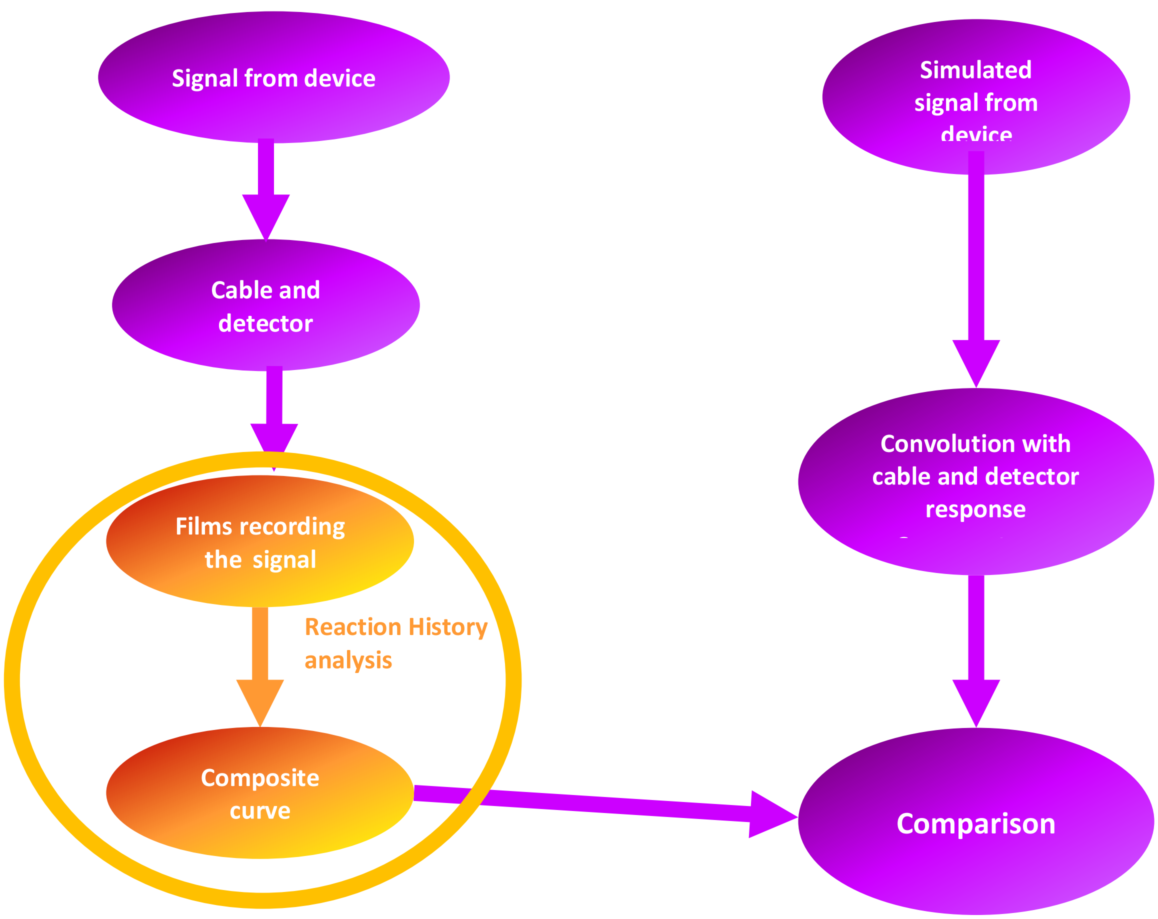

Fig. 1 Comparison between measured and simulated device signal

Deconvolution is a mathematically ill-posed problem. Numerically, deconvolution of two experimental, noisy functions significantly amplifies noise. For these reasons the experimental reaction history composite curve needs to be compared with simulations' results that are convolved with detector and cable response functions. This method of comparison limits uncertainty yet is not uncertainty-free.

Fig 1. presents a multi-step process of measuring experimental reaction history generated by a device, analyzing the data, and comparing the data with results of simulations convolved with cable and detector response functions. It has independent sources of uncertainties; all of them need to be accounted for, when a comparison between experimental data and simulations are performed.

There are multiple sources of uncertainty of cable and detector response functions. The effect of cable response and limitations of the cable bandwidth are much more important than detector response. We need to consider uncertainty of cable response files that are used.

Convolution does not amplify the experimental uncertainty as much as the deconvolution, yet still uncertainty of the convolved function needs to be considered.
Numerical study performed by Mike Ham in 2016 showed that in some portions of the alpha curve uncertainty of convolved function caused by cable response uncertainty was well under 1%, in other portions of the same curve it was about 5%, yet in one important region of the curve uncertainty defined in the same way was about 20%. General causes of these non-intuitive numerical results are that limitations of the cable bandwidth affects different portions of the alpha curve differently; and that convolution is a non-local transformation. It requires further study.

Propagation of uncertainty from flux to α

Let's discuss propagation of uncertainty from flux to α. The flux and the α are functions of time, so the notation for them is $f(t)$ and $\alpha(t)$, respectively.

The flux has uncertainty which we call$\Delta f(t)$, and assume it is symmetric. The rationale for that assumption is that the uncertainly in the flux is assumed Gaussian and thus symmetric by the reaction history Loco program and the Monte Carlo routines it uses.

1) Definition of $\alpha(t)$:

$$\alpha(t) \coloneqq \frac{d}{dt} \ln f(t)$$

Thus

$$\alpha(t) = \frac{\dot{f}(t)}{f(t)}$$

where $\dot{f}(t) = \frac{df(t)}{dt}$

Introducing notation $\dot{\Delta f} \coloneqq \frac{d}{dt}\Delta f(t)$

we get, in accordance with the above definition and functional dependence of $\alpha(t)$ that the uncertainty in $\alpha(t)$, denoted $\Delta\alpha$, achieved in the upper and lower limits of the flux should satisfy

$$\alpha \pm \Delta\alpha = \frac{d}{dt}\ln(f \pm \Delta f) = \frac{\dot{f} \pm \dot{\Delta f}}{f \pm \Delta f}$$

Let's discuss the propagation of the uncertainty in special cases.

2) Calculation of uncertainty propagation in the case when the flux has systematic uncertainty of the form $\Delta f = \varepsilon f$, ε a constant

   In this case

$$\alpha \pm \Delta\alpha = \frac{d}{dt}\ln(f \pm \varepsilon f) = \frac{d}{dt}\ln\big((1 \pm \varepsilon)f\big) = \frac{d}{dt}[\ln(1 \pm \varepsilon) + \ln f] = \frac{d}{dt}\ln f$$

   As a result, the propagated uncertainty in α, $\Delta\alpha_{\varepsilon} = 0$. In other words, when systematic uncertainty in the flux f is of the form $\Delta f = \varepsilon f$, with constant ε, the uncertainty does not propagate to α, even for large ε.

3) Calculation of uncertainty propagation in the case when the flux has general systematic uncertainty $\Delta f(t)$, under the assumption that the uncertainty in the flux is small in comparison to the flux itself, $\Delta f(t) \ll f(t)$.

   Using the approximation, true to the second order in $\Delta f(t)$,

$$\frac{1}{f \pm \Delta f(t)} \approx \frac{1}{f}$$

   we get

$$\alpha \pm \Delta\alpha_{appx} \approx \frac{\dot{f} \pm \dot{\Delta f}}{f} = \frac{\dot{f}}{f} \pm \frac{\dot{\Delta f}}{f} = \alpha \pm \frac{\dot{\Delta f}}{f}$$

   where the approximate equality means equality up to second order in the small quantity $\frac{\Delta f}{f}$.

   As a result, the propagated uncertainty in α is equal to (again approximate equality means equality up to second order expression in $\frac{\Delta f}{f}$)

$$\Delta\alpha_{appx} \approx \frac{\dot{\Delta f}}{f}$$

4) General $\Delta f(t)$ (no assumption of smallness of uncertainty in the flux or any relationship of the uncertainty in flux with the flux).

The formula for uncertainty propagation from the flux to α gives

$$\Delta\alpha_{\pm} = \alpha(f \pm \Delta f) - \alpha(f) = \frac{\dot{f} \pm \Delta\dot{f}}{f \pm \Delta f} - \frac{\dot{f}}{f} = \frac{f\dot{f} \pm f\Delta\dot{f} - f\dot{f} \mp \Delta f\dot{f}}{f(f \pm \Delta f)} = \frac{\pm f\Delta\dot{f} \mp \Delta f\dot{f}}{f(f \pm \Delta f)}$$

In other words, after dividing the numerator and denominator by f, we get

$$\Delta\alpha_{+} = \frac{\Delta\dot{f} - \Delta f\frac{\dot{f}}{f}}{f + \Delta f} = \frac{\Delta\dot{f} - \Delta f\alpha}{f + \Delta f}$$

$$\Delta\alpha_{-} = \frac{-\Delta\dot{f} + \Delta f\frac{\dot{f}}{f}}{f - \Delta f} = \frac{-\Delta\dot{f} + \Delta f\alpha}{f - \Delta f}$$

5) Some relations between above uncertainties

a. Since for $\alpha > 0$, $f > 0$, $\Delta f > 0$, we have $\Delta f\alpha > 0$ and $\frac{1}{f+\Delta f} < \frac{1}{f}$ then

$$\Delta\alpha_{+} = \frac{\Delta\dot{f} - \Delta f\alpha}{f + \Delta f} < \frac{\Delta\dot{f}}{f} = \Delta\alpha_{appx}$$

b. Due to the following series of equalities

$$\Delta\alpha_{-} = \frac{-\Delta\dot{f} + \Delta f\alpha}{f - \Delta f} = -\frac{1}{f - \Delta f}\left(\Delta\dot{f} - \Delta f\alpha\right) = -\frac{1}{f - \Delta f}(f + \Delta f)\Delta\alpha_{+}$$

$$= -\Delta\alpha_{+}\left(1 + \frac{2\Delta f}{f - \Delta f}\right) = -\Delta\alpha_{+}\left(1 + \frac{2}{\frac{f}{\Delta f} - 1}\right)$$

we have the following inequality

$$|\Delta\alpha_{-}| > |\Delta\alpha_{+}|$$

c. We have also

$$\Delta\alpha_{appx} + \Delta\alpha_{-} = \frac{\Delta\dot{f}}{f} + \frac{-\Delta\dot{f} + \Delta f\frac{\dot{f}}{f}}{f - \Delta f} = \frac{f\Delta\dot{f} - \Delta f\Delta\dot{f} - f\Delta\dot{f} + \Delta f\dot{f}}{f(f - \Delta f)}$$

$$= \frac{\Delta f\left(\dot{f} - \Delta\dot{f}\right)}{f(f - \Delta f)} = \frac{\Delta f}{f}\frac{d}{dt}\ln(f - \Delta f)$$

Since $\Delta f > 0$, $f > 0$, and $\frac{d}{dt}\ln(f - \Delta f) > 0$, the latter inequality following from the fact it represents an α, which must be positive,

$$\Delta\alpha_{appx} + \Delta\alpha_{-} > 0$$

As a result of the latter inequality, we have

$$\Delta\alpha_{appx} > |\Delta\alpha_{-}|$$

Summarizing inequalities obtained in a-c, we can write the following relation between the different uncertainties

$$\Delta\alpha_{appx} > |\Delta\alpha_{-}| > |\Delta\alpha_{+}|$$

Systematic Uncertainty

There are always multiple sources of uncertainty of an experimentally measured quantity that effectively can be accounted for by a systematic uncertainty. The sources of uncertainty in this case are connected to the detector, cables, and the recording system. They are also caused by the film reading uncertainties like uncertainty in assigning the baseline. All of them are affecting flux – the experimentally measured quantity. Systematic uncertainties are proportional to the measured value:

$$\Delta f = \varepsilon f$$

Then

$$\boldsymbol{\frac{d}{dt}\ln[(1+\varepsilon)f] = \frac{(1+\varepsilon)\dot{f}}{(1+\varepsilon)f} = \frac{\dot{f}}{f} = \alpha(f)}$$

Therefore, ***no systematic uncertainty propagates from the flux to α.***

Summary and Path Forward

The scope of the uncertainty of the reaction history data analysis is discussed in detail in order to define clearly what this uncertainty includes, and what it does not include.

Uncertainty of experimental measurement is independent from the physics governing reproducibility of an experiment.

In the current reaction history reanalysis we do not de-convolve the composite curve. Simulation results are convolved with detector and cable response functions for comparison with the experimental composite curve. Uncertainties of simulations convolved with the detector and cable responses need to be studied. According to current, rather preliminary assessment, these uncertainties are comparable to uncertainties propagated from the flux to α. They may even be the dominant ones.

Gamma flux as a function of time is an experimental quantity, measured by a set of reaction history detectors. But alpha as a function of time is a quantity derived from the flux - it is a time derivative of logarithm of the flux. ***Experimental measurement uncertainty, including any kind of systematic uncertainty in such measurement is generated exclusively for the flux***.

We have shown here why ***systematic uncertainty is not propagated from the flux α.***

Other kinds of uncertainty are propagated to the alpha, the formulas are included in these notes.
These notes present mathematical approach to the reaction history alpha uncertainty. Software implementation is documented separately. It is worthy to consider if the numerical implementation in the current reaction history software is optimal or are there areas for improvement.